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What is it that analytical chemists do?

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Her future goal is to found a centre for chemical information science and technology as a joint venture with partners from science and industry.

If I want to draw public attention to our field of research and our products, that is, if I go public, I have to explain to lay people and investors what our aims are in an informative and easily digestible way. I need to use examples and, even more importantly, a language everybody can understand. What is it, then, that we do every day in Analytical Chemistry?

Gary M. Hieftje called our discipline “the science of measurements and instrumentation” [1]. Royce W. Murray cited a claim by president Bruce Alberts of the National Academy of Science in the USA: “What is measured in high-stakes assessments has a profound effect on human behavior” and a corollary: “We must be exceedingly careful to make sure that we measure what counts” [2]. The first quotation is certainly correct and relevant, and in synergy with Bruce Alberts claim and corollary.

In line with these statements, the following examples show that if Analytical Chemistry did not already exist, it would have to be invented immediately. Without Analytical Chemistry it would not be possible to trace BSE antibodies, to quantify glucose in blood specimens, or pesticides, herbicides, VOCS, TOC¹, and heavy metals in environmental specimens. The progress made in clinical chemical analysis since my first steps in the field in 1968 has been enormous, and I agree with Renato Zenobi when he says that we should be proud to be Analytical Chemists (“Chin up, Chest out” [3]). I do, nevertheless, feel somewhat helpless if I have to explain to a lay person what it is we analytical chemists actually do.

Talking about “analysis” implies dealing with a major branch of mathematics, psychology, or business strategies. “Chemistry and chemical compounds” tend to be viewed negatively by the public so I try to avoid the terms. In sensor research, in particular, I claim to work or measure “without using chemical reagents”. This is especially important if the chemical information to be ob-

¹VOCs, volatile organic carbons; TOC, total organic carbon.

tained is related to the life sciences and to the medical and biological environments. Finally, why should we have to make use of chemical compounds at all to measure something? There are many other ways of measuring a quantity!

In the end I came to the conclusion that what all types of technology in Analytical Chemistry have in common is that they aim to obtain *chemical information about the state of a source so that this information can be used to make decisions*. For decision making the result of chemical analysis must be linked with the expert decision by an information chain. This information chain is: determination; interpretation; and action. The action is the consequence of a cut-off value including a range of uncertainty set as a decision limit. By applying cut-off values, the analytical results are reduced to a binary scale. This procedure is well-known in medical diagnosis and environmental monitoring. Such an information chain is the basis of any process or bioprocess to be controlled on the basis of results of a continuous monitoring system. The cut-off values are not necessarily values of a single quantity, however, but rather of a set of quantities which enable imaging of the process in the virtual environment. With "chemical information systems" installed close to the source (*on line, in line, at line*), a cost-effective strategy for process control can be developed on the basis of an optimized and effective strategy of chemical analysis. Let me give an example.

The chemical analysis system might be a system incorporating an array of chemical sensors which serves to yield *chemical information*. For continuous monitoring close to the source highly automated chemical analysis is necessary. The results should enable reproduction of the chemical processes at the source in a virtual environment. The accuracy of the analytical data is guaranteed by periodic, automated recalibration. Expert decisions are, in this instance, based on the results of the sensor array, multivariate data analysis, data reduction, and data presentation, not to mention expert systems capable of validating and interpreting data. For bioprocesses, the chemical target compounds are termed "biomarkers". Such biomarkers are feed compounds and metabolites such as carbohy-

drates, ammonia, nitrite, nitrate, amines, alcohols, acetate, anions, and cations such as magnesium ions. The transient activity of these biomarkers enables the state of a biological system (reproduction of cells, growth inhibition, steady-state) to be described. It enables the process to be optimized by feed-back control and, in addition, information to be obtained on toxic species, for example heavy metals, cyanide, etc. By using the term "biomarkers", I avoid speaking about "chemical compounds".

Because we are in the information technology millennium, we can expect most people to understand the term "chemical information" derived from the results yielded, and "chemical information systems" and "chemical information units" denoting the measuring systems. It might well be that in chemical sensor research and process analysis plausible explanations of our activities are even harder to give than in other fields of Analytical Chemistry. I will, nevertheless, use the term "Chemical Information Technology" in my next presentations and talk about research in "Chemical Information Science". I will use the term "biomarkers" to refer to the analytes or chemical compounds to be analyzed in biological processes which are related to the chemistry of C, H, N, O, S, and to the vital salts and trace elements.

By using these terms we can begin to show how Analytical Chemistry is relevant to society in the sense of: "What is measured in high-stakes assessments has a profound effect on human behavior." and "We must be exceedingly careful to make sure that we measure what counts." Having these claims in mind, we will feel inclined to present a *diagnosis of a source* rather than analytical data. At the Centre for Chemical Sensors/Biosensors and bioAnalytical Chemistry we are offering tools which are able to solve problems in *Chemical Information Science and Technology*.

References

1. Hieftje GM (2000) Anal Chem 72:309A
2. Murray RW (1997) Anal Chem 69:443A
3. Zenobi R (2000) Anal Chem 72:245A